Subject: Re: Converting COD2020 to SDF
Posted by nbehrnd on Fri, 29 Jan 2021 18:59:25 GMT
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Coincidental side note: Crystallographic data as basis to set up force fields is a centre of gravity of Hofmann's chapter about small organic molecules in «Data Mining in Crystallography» within the series «Structure and Bonding»:

https://link.springer.com/chapter/10.1007/978-3-642-04759-6_ 4

Norwid